

4H-Pyran, 4-(2,6-diphenyl-4H-pyran-4-ylidene)-2,6-diphenyl-

Other names: Bipyranylidene, 2,2',6,6'-tetraphenyl-
Inchi: InChI=1S/C34H24O2/c1-5-13-25(14-6-1)31-21-29(22-32(35-31)26-15-7-2-8-16-26)30-23
InchiKey: YXUHEZNMKMTXME-UHFFFAOYSA-N
Formula: C34H24O2
SMILES: C1=C(c2ccccc2)OC(c2ccccc2)=CC1=C1C=C(c2ccccc2)OC(c2ccccc2)=C1
Mol. weight [g/mol]: 464.55
CAS: 42506-57-0

Physical Properties

Property code	Value	Unit	Source
gf	669.14	kJ/mol	Joback Method
hf	306.43	kJ/mol	Joback Method
hfus	61.24	kJ/mol	Joback Method
hvap	116.31	kJ/mol	Joback Method
ie	5.80	eV	NIST Webbook
log10ws	-10.35		Crippen Method
logp	8.508		Crippen Method
mcvol	363.400	ml/mol	McGowan Method
pc	1467.98	kPa	Joback Method
tb	1212.06	K	Joback Method
tc	1511.95	K	Joback Method
tf	733.92	K	Joback Method
vc	1.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1186.46	J/mol×K	1212.06	Joback Method
cpg	1198.71	J/mol×K	1262.04	Joback Method
cpg	1210.37	J/mol×K	1312.02	Joback Method
cpg	1221.74	J/mol×K	1362.01	Joback Method
cpg	1233.15	J/mol×K	1411.99	Joback Method
cpg	1244.91	J/mol×K	1461.97	Joback Method
cpg	1257.35	J/mol×K	1511.95	Joback Method

dvisc	0.0001044	Pa×s	733.92	Joback Method
dvisc	0.0000608	Pa×s	813.61	Joback Method
dvisc	0.0000389	Pa×s	893.30	Joback Method
dvisc	0.0000268	Pa×s	972.99	Joback Method
dvisc	0.0000196	Pa×s	1052.68	Joback Method
dvisc	0.0000149	Pa×s	1132.37	Joback Method
dvisc	0.0000118	Pa×s	1212.06	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C42506570&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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